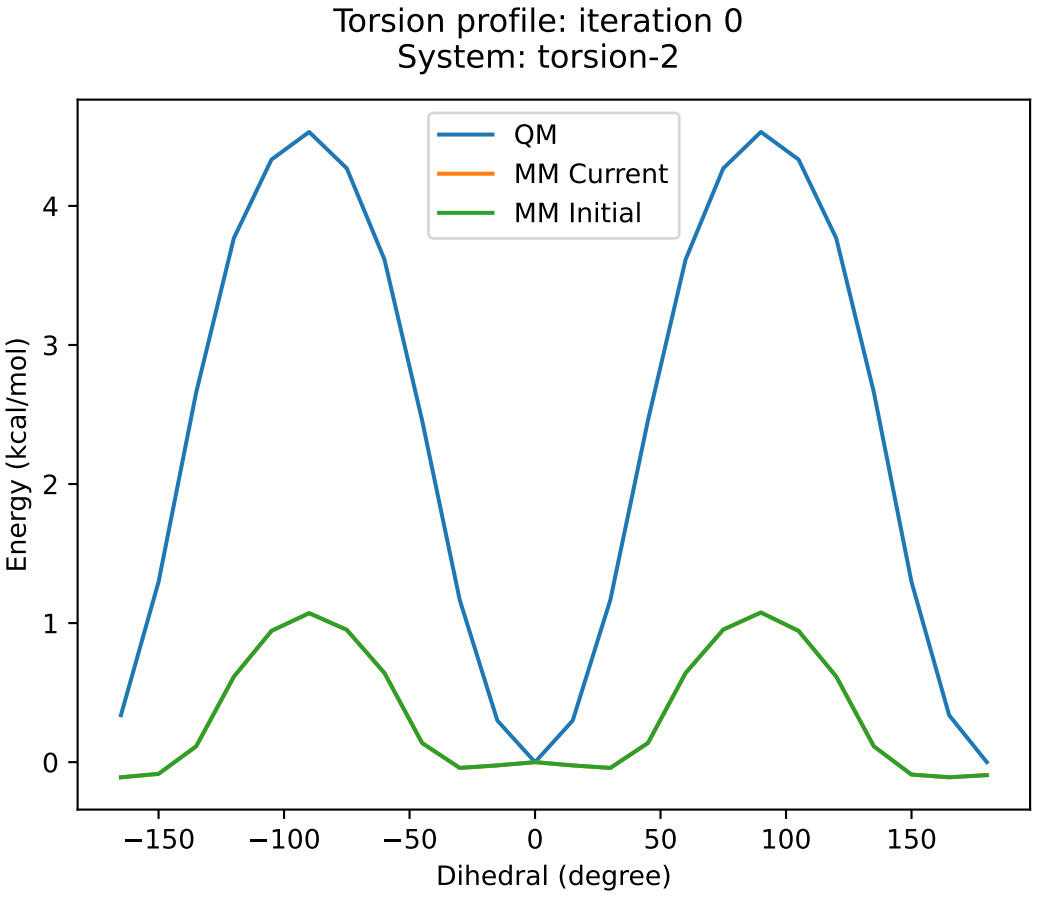
Torsion profile: iteration 0
System: torsion-2
QM
MM Current
MM Initial
Energy (kcal/mol)
0
1
2
3
4
−150
−100
−50
0
50
100
150
Dihedral (degree)